BIO-315

Biomolecular structure and mechanics

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Cursus	Sem.	Type
Biocomputing minor	E	Opt.
Bioengineering	MA4	Opt.
Computational science and Engineering	MA2, MA4	Opt.
Life Sciences Engineering	MA2, MA4	Opt.
Sciences du vivant	MA4	Opt.

Language of teaching	English
Credits	4
Session	Summer
Semester	Spring
Exam	During the semester
Workload	120h
Weeks	14
Hours	**4 weekly**
Lecture	2 weekly
Exercises	2 weekly
Number of positions	

Summary

Main focus of this course is on the description and design of molecular interactions defining the structure, dynamics and function of biological systems. The principal experimental and computational techniques used in structural biology, molecular modeling and design will be introduced and practiced

Content

1. Structure: intermolecular interactions, structure of biomolecules, experimental methods in structural biology (X-ray crystallography, NMR, cryo-electron microscopy), structural classification, comparative modeling, protein structure prediction using genomic data and machine learning.
2. Dynamics: elements of statistical mechanics, molecular mechanics of biomolecules, molecular dynamics simulations, binding and free energy calculations.
3. Selected topics: protein design and engineering; protein folding, protein docking, integrative modeling; structure-based drug discovery, multiscale molecular simulation techniques.
Practicals and projects will run in parallel to lectures to have a first-hand experience on molecular visualization, X-ray crystallography, molecular modeling tools applied to protein structure prediction and design, biomolecular mechanics and dynamics, structure-based drug design, proteome-wide prediction of protein interaction networks, protein folding games (Foldit).

Keywords

Structural biology, X-ray crystallography, cryo-EM, NMR, SAXS, integrative modeling, molecular modeling, molecular mechanics, molecular simulation, protein structure prediction, protein folding, protein design, drug discovery.

Learning Prerequisites

Recommended courses

Basic bachelor courses of Mathematics, Physics, Molecular Biology and Biochemistry

Important concepts to start the course

Structural biology and biochemistry of proteins, nucleic acids and membranes. Classic mechanics, themodynamics, and electrostatics (Physics I, II, III).

Learning Outcomes

By the end of the course, the student must be able to:

- Explore the structure of biomolecules (and their interactions)

- Predict and design the structure & dynamics of proteins
- Work out / Determine the structure of biomolecules
- Perform X-ray crystallography experiments
- Perform molecular modeling and simulation
- Choose the appropriate method to tackle a problem
- Design a project in structural biology
- Make a scientific report and presentation
- Assess / Evaluate the role of intermolecular interactions in biology
- Conduct X-ray crystallography experiments

Transversal skills

- Set objectives and design an action plan to reach those objectives.
- Assess one's own level of skill acquisition, and plan their on-going learning goals.
- Assess progress against the plan, and adapt the plan as appropriate.
- Continue to work through difficulties or initial failure to find optimal solutions.
- Use both general and domain specific IT resources and tools
- Make an oral presentation.
- Write a scientific or technical report.

Teaching methods

Half of the course is based on lectures, while in the other half practical experiences and projects (computational and experimental) are provided to the students.

Expected student activities

Attending lectures, completing practical experiences, reading assignments, presenting a scientific paper, doing a project, writing a report, presenting the results of a project

Assessment methods

Projects assessment during the semester

Supervision

Office hours	Yes
Assistants	Yes
Forum	Yes

Resources

Bibliography

Molecular modelling: principles and applications, A.R. Leach, Pearson
Molecular modeling and simulations, T. Schlick, Springer

Ressources en bibliothèque

- Molecular modelling / Leach
- Molecular modeling and simulations / Schlick

Notes/Handbook

Lecture slides and exercises are provide via moodle.

Moodle Link

- http://moodle.epfl.ch/enrol/index.php?id=6741